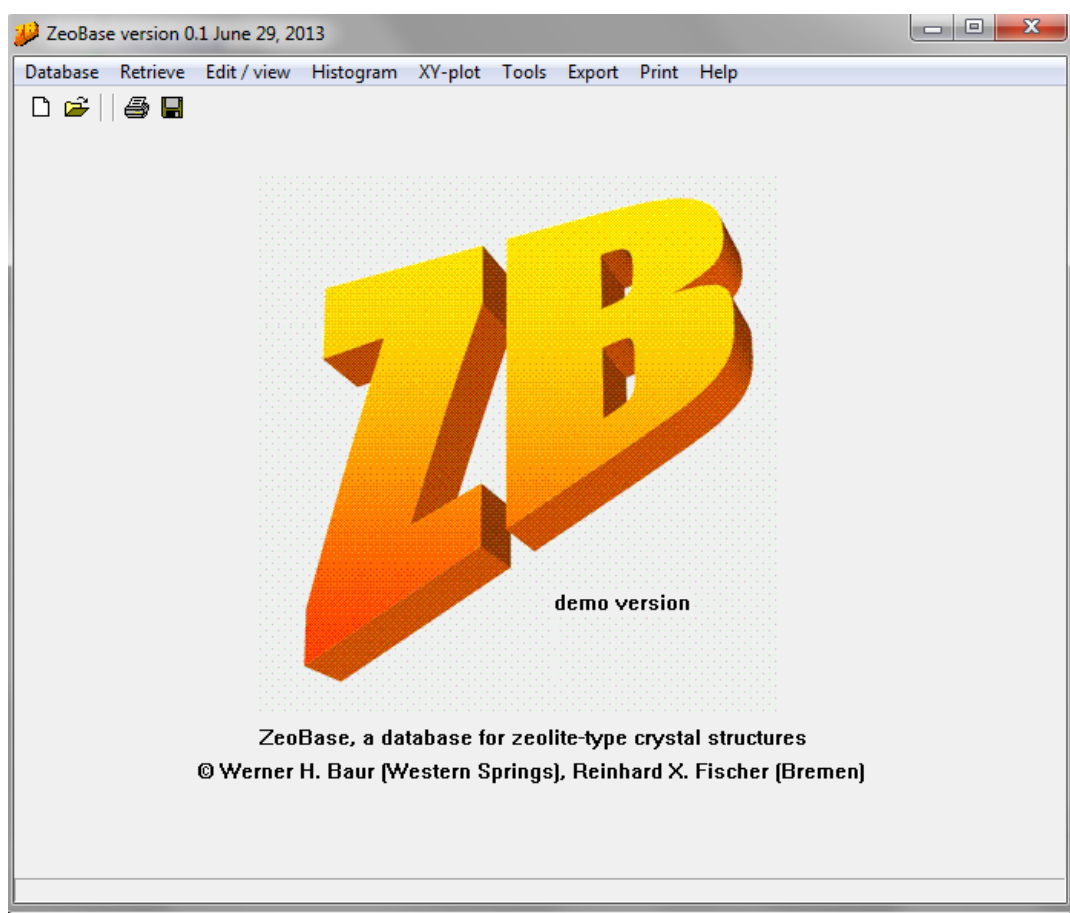


ZeoBase, a database for zeolite-type crystal structures

User manual

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beta-version July 2013



1.	Introduction	3
1.1	General information.....	3
1.2	Database contents	3
1.3	Standardized crystal data	3
1.4	Licensing and Copyright, © 2013 by Werner H. Baur and Reinhard X. Fischer.....	6
1.5	Disclaimer.....	7
2.	Installation of ZeoBase.....	7
3.	Program handling	8
3.1	Starting ZeoBase.....	8
3.2	Retrieve options.....	9
3.2.1	Overview	9
3.2.2.	Framework type code (FTC).....	9
3.2.3	Zeolite Name	10
3.2.4	Bibliographic data	10
3.2.5	Keywords	11
3.2.6.	Chemical composition.....	13
3.2.7	Unit-cell parameters	13
3.2.8	Framework density	14
3.2.9	Space-group symmetry.....	14
3.2.10	Distances and angles	15
3.2.11	Crystal system	15
3.3	List of selections	16
3.4	Edit/view menu.....	18
3.4.1	Overview	18
3.4.2	Bibliographic data	18
3.4.3	Crystal data.....	19
3.4.4	Lattice parameters, Atomic coordinates, Atomic coord. HTML, Sample data, Comments, TO distances, TO dist HTML table	20
3.4.5	Zeobase.out, zeograph.out.....	20
3.5	Histograms.....	20
3.6	XY-plots	22
3.7	Tools	24
3.7.1	Distances and angles	24
3.7.2	SADIAN.....	24
3.7.3	STRUPLO	24
3.7.4	Powder pattern.....	24
3.7.5	BRASS	25
3.8	Export	25
3.8.1	cif.....	25
3.8.2	SADIAN.....	25
3.8.3	STRUPLO	25
3.8.4	Save active frame	25
3.9	Print	25
3.10	Help.....	25
4.	References	26
5.	Appendix	27
5.1	Journal codes	27
5.2	Hot keys (shortcuts).....	32
5.3	File assignments	33

1. Introduction

1.1 General information

ZeoBase is a database for crystal chemical data of compounds with zeolite-type crystal structures. It currently contains more than 5,500 entries of crystal-structure determinations. For more than 4,700 of them the complete crystallographic information is available (space group, unit-cell dimensions, atomic coordinates, chemical composition) and it includes comments concerning the sources of the studied samples. In addition, within each zeolite framework type all entries are fully standardized (see 1.2). The standardization procedure allows the easy comparison of structural parameters and the unambiguous assignment of framework atoms to their sub- and supergroup counterparts, without being limited by space-group symmetry or settings [1-3]. Thus this set of crystal structure data provides information uniquely useful for the correlation of a host of structural and physico-chemical relationships.

Crystal structure data have been compiled by us for more than twenty years. We strive for a complete collection of all available crystal-structure determinations of zeolites. Presently, ZeoBase encompasses more zeolite entries than any other database. About **50%** of the entries are edited, corrected, or emended in a review process, that is documented in comments accessed in Edit/view (see 3.4.4). *ZeoBase* is an evaluated compilation.

Crystal-structure data are entered into ZeoBase whenever the published information is sufficient to calculate the bond distances and angles for the structure and/or a powder pattern can be obtained. If certain data are missing in the original papers for these purposes they are supplied either by contacting the original authors or by guessing the requisite data from the internal evidence of the papers whenever this is possible.

Crystal and chemical data can be correlated and displayed in histograms or XY-plots. This is made possible by the standardization of crystal data comprising unit-cell settings, sequence of atoms, and atom names.

1.2 Database contents

ZeoBase is searchable for the following properties: zeolite name, framework-type code, author, year of publication, unit-cell parameters and volume, framework density, space group, crystal system, T-O distances and their estimated standard deviations (e.s.d.), T-O-T and O-T-O angles and their e.s.d.'s, and most importantly for the chemical elements present in the zeolites. In addition, up to 23 keywords can be selected to specify sample properties and experimental conditions. The results, where appropriate, can be displayed as tables, plots or histograms. Since the names and labels of all individual atoms in each of the topologically identical crystal structures are standardized one can follow particular bond lengths or bond angles in their symmetry-related changes from zeolite to zeolite. In addition, tools are provided to display various properties, such as framework density, mean bond lengths or angles, individual bond lengths or angles or chemical composition [4]. This is useful for studying the flexibility of zeolites as a function of their geometry, their topology or their chemistry. In addition one can see which zeolites can accommodate which atoms within their frameworks or which frameworks can tolerate which exchangeable atoms within their pores [4].

1.3 Standardized crystal data

All crystal structure entries are standardized by conforming to selected entries which usually represent the most prominent member within the FTC structural family. Generally applied standardization routines, such as Structure Tidy [5,6] cannot be used for this purpose because they standardize unit-cell settings and atomic coordinates just within a given space

group and do not consider structural relationships between related phases crystallizing in different space groups. The use of such a program would yield different settings with different origins in various group-subgroup relationships and would result in a different ordering of atoms in many space groups which, in fact, should be in the same setting and in the same order throughout all the space groups listed within a Bärnighausen tree [7]. The standardization procedure introduced here enables us to directly compare the crystal structures occurring in different space groups and to discuss the local environments of the atoms independent of their representation in the original literature.

In some cases it was necessary during the standardization procedure to transform the crystal structures via a mirror plane or a center of inversion, thus inverting basis vectors of the unit cell. Unless the authors stated explicitly that the absolute configuration of the crystal structure had been determined, we assumed that the original description of the crystal structures corresponded to an arbitrary choice in the crystal structure analysis.

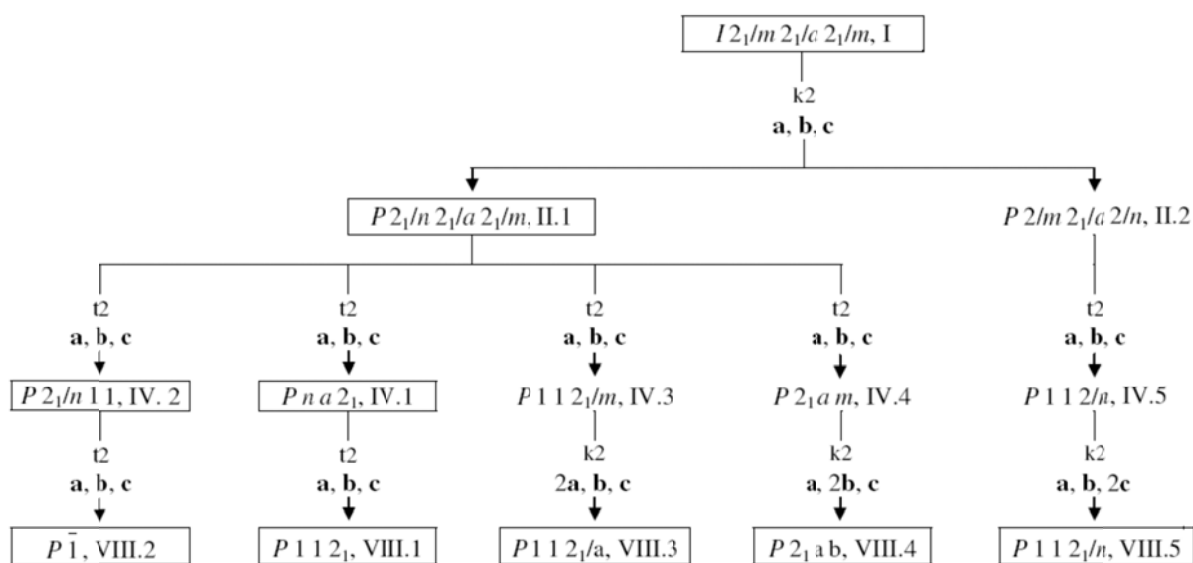


Fig. 1.3.1: The Bärnighausen tree [7] for ABW-type frameworks (from ref. [8]).

A standard setting for the aristotypic structure (structure with highest symmetry for a specific framework type) is selected from the space group with the highest number of entries, thus representing the most prominent structures. In the case of ABW-type structures (Fig. 1.3.1), the space group with the highest number of entries is $Pn\bar{a}m$. The highest possible symmetry in this group is $Im\bar{m}a$ represented in the $Im\bar{m}a$ setting to conform to $Pn\bar{a}m$. The atomic parameters in the aristotype structure are given in two groups, the group of framework cations (labeled T for tetrahedrally coordinated atoms) and the group of framework anions (labeled O after oxygen as the most prominent anion in zeolites). Within the two groups, the sequence of atoms follows the sequence of Wyckoff symbols for the respective space group after International Tables, going from lowest to highest symmetry (highest to lowest multiplicity) as shown in Fig. 1.3.2 for the ABW aristotype.

ABW-I <i>I m a m</i>	ABW-II <i>P n a m</i>	ABW-IV.1 <i>P n a 2₁</i>	ABW-VIII.1 <i>P 1 1 2₁</i>
T1 [8(i), ... m]	T11 [4(c), ... m] T12 [4(c), ... m]	T11 [4(a), 1] T12 [4(a), 1]	T11a [2(a), 1] T11b [2(a), 1] T12a [2(a), 1] T12b [2(a), 1]
O1 [4(e), <i>m</i> 2 <i>m</i>]	O1 [4(c), ... m]	O1 [4(a), 1]	O11 [2(a), 1] O12 [2(a), 1]
O2 [4(c), ... 2/ <i>m</i>]	O2 [4(c), ... m]	O2 [4(a), 1]	O21 [2(a), 1] O22 [2(a), 1]
O3 [8(f), 2 ...]	O3 [8(d), 1]	O31 [4(a), 1] O32 [4(a), 1]	O31a [2(a), 1] O31b [2(a), 1] O32a [2(a), 1] O32b [2(a), 1]

Fig. 1.3.2 Atomic site relationships in branch 1 of Fig. 1.3.1 (from ref. 1).

All derivatives of this standard member in supergroups and subgroups adopt the same setting of the space group irrespective of the standard setting in the International Tables (IT, [9]). The sequence of atoms within an entry of a subgroup strictly follows the sequence of atoms in the aristotype.

The complete group-subgroup relationships are illustrated by Bärnighausen trees [7]. All space groups are given as maximal subgroups derived from the space group representing the highest possible topological symmetry. Branches contain information on the type of the subgroup relationship (translationengleich or klassengleich) with the respective subgroup index representing the factor of the symmetry reduction or the number of cosets derived from the supergroup. Furthermore, the set of basis vectors is given which describes the transformation of a unit cell to its setting in the subgroup. The hierarchical order of the space groups is represented by Roman numerals assigned to the space group symbols. The aristotype has always the number I, the subgroups have numerals corresponding to their index of symmetry reduction relative to the aristotype. Entries with the same index are always drawn on the same height, thus representing members of the same hierarchical order. Members on one level occurring in different branches are distinguished by Arabic numerals. Space groups representing observed crystal structures are put in frames. Space groups presented without frames are needed to indicate intermediate steps in describing symmetry transformations. Likewise the aristotypic space groups are shown without a frame whenever they are not observed because they do not allow an ordered distribution of different cations on the T-sites.

In some cases Bärnighausen trees with alternative branches would be possible in order to describe a symmetry derivation. In these cases, those intermediate subgroups are selected which allow an ordered distribution of different T-atoms as observed in the lower symmetry. If there is more than one space group to describe this derivation, the space group is selected arbitrarily, usually representing the simplest derivation.

The atomic site relationships are tabulated based on the derivations in the Bärnighausen tree. Arrows indicate the splitting of atom sites upon symmetry reduction, which is usually an ordering process for the framework cation sites. Wyckoff positions and site symmetries are given in square brackets according to the notation in the International Tables for Crystallography [9]. Atom names are derived from the corresponding names in the aristotype, keeping the numeral assigned to the atom in its highest symmetry and adding a second numeral expressing the second level derivation. If an atom site is not affected by the symmetry reduction, it keeps the name of its supergroup root name. Upon further reduction of the symmetry, lower case letters are added to the atom names.

The above information is given as background for the understanding of the treatment of the data in ZeoBase. Bärnighausen trees and atomic site relationships are implicit in ZeoBase. They are explicitly presented in the cited literature [1-3, 8].

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2. Installation of ZeoBase

The demo version of ZeoBase is distributed on a CD and can be installed without any copy protection. The full version will be distributed on CD as well. However, it can be installed and run only with a dongle supplied after signing a contract for a one-year license.

Database, user interface, and program tools like STRUPLO and BRASS are packed into a single installation routine named “setup_ZeoBase.exe”. The installation is started by double click on “setup_ZeoBase.exe”. Perhaps you will be prompted by your system if any protection software is active to control changes in the windows registry. In that case, allow modifications by clicking “yes” or any corresponding options. Then, the installshield wizard for ZeoBase will be started. Follow the instructions and accept all terms for license agreements. By default, ZeoBase programs are installed on c:\program files (or equivalent on various windows operating systems) by creating a subdirectory ZeoBase. This could be modified if requested by pressing the “change...” button. All data accessed by ZeoBase are written on a subdirectory of c:\program files\ZeoBase named “Database”. After finishing the installation, all programs and data are accessible with an icon placed on the desktop and an entry in the windows startup program menu. However, it is strongly recommended to create a separate directory for all input and output files generated by ZeoBase, preferably on another partition of the hard disk (usually d:\ or e:\).

3. Program handling

3.1 Starting ZeoBase

There are three ways of starting ZeoBase: (1) Doubleclick on the desktop icon , (2) select ZeoBase in the windows program start menu, (3) doubleclick on "ZeoBase_yyyy-mm-dd.exe" in "c:\program files\ZeoBase" (or equivalent) where yyyy-mm-dd stands for the date (year, month, day) of the actual program version. The main menu as shown in Fig. 1 will appear.

Before using ZeoBase, the working directory must be created by selecting "new" (short-cut: CNTL+N) in the Database menu or, if it already exists, by selecting "open" (short-cut: CNTL+O). Alternatively the corresponding icons   can be accessed directly.

Most of the active frames can be printed or saved to a file by clicking on icon  or . Alternately, the respective commands in pull-down menus export and print can be used as well as shortcuts Ctrl+P and Ctrl+S. In the demo version, printing and saving is only possible by selecting the icons on the main frame (Fig. 3.1.1) or using the above mentioned shortcuts if the main frame is the active frame.

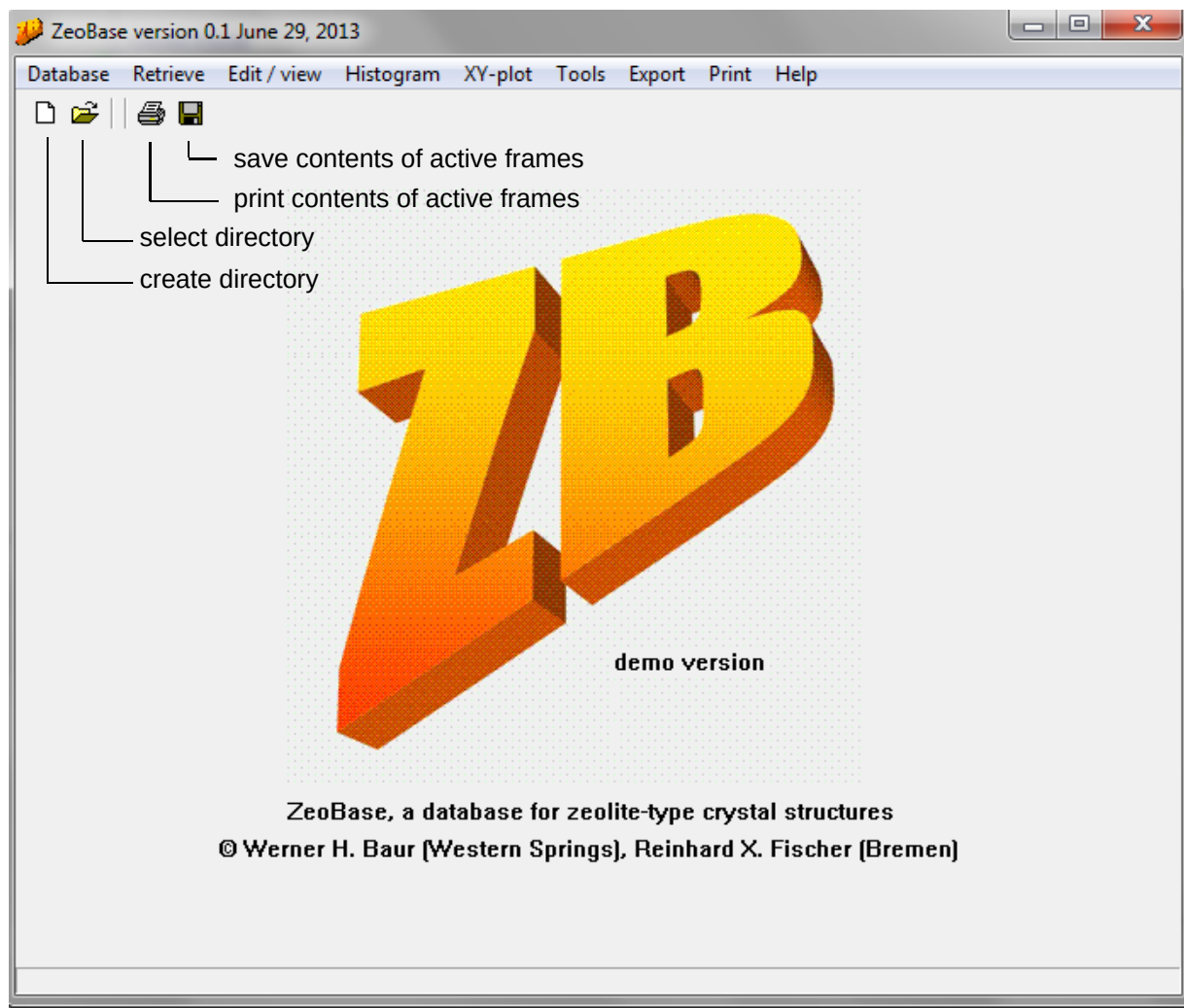


Fig. 3.1.1: Main menu

3.2 Retrieve options

3.2.1 Overview

Retrieve	Edit / view	Histogram	XY-plot
FTC			
Zeolite name			
Bibliographic data			
Key words			
Chemical composition			
Unit cell parameters			
Framework density			
Symmetry			
Distances and angles			
Crystal system			
temperature and pressure			

ZeoBase has a retrieval system (Fig. 3.2.1) selecting entries by framework-type codes (FTC), zeolite names, author names or year of publication in "Bibliographic data", key words, chemical composition, unit-cell parameters, framework density, space group symbol or space group number, interatomic distances and angles, crystal system, and finally temperature and pressure at syntheses and data-collection conditions. Corresponding shortcuts are listed in Fig. 3.2.1. In all submenus, the boolean operators "and", "or", and "not" can be selected to define conditions for the retrieval of entries. Default is "or". If another operator should be applied it must be pressed prior to the selection of items. The color of the selected items will be changed to green for "or" operations, blue for "and", and red for "not". The retrieve menu contains 11 tab sheets appearing after selecting any of the options shown in Fig. 3.2.1.

3.2.2. Framework type code (FTC)

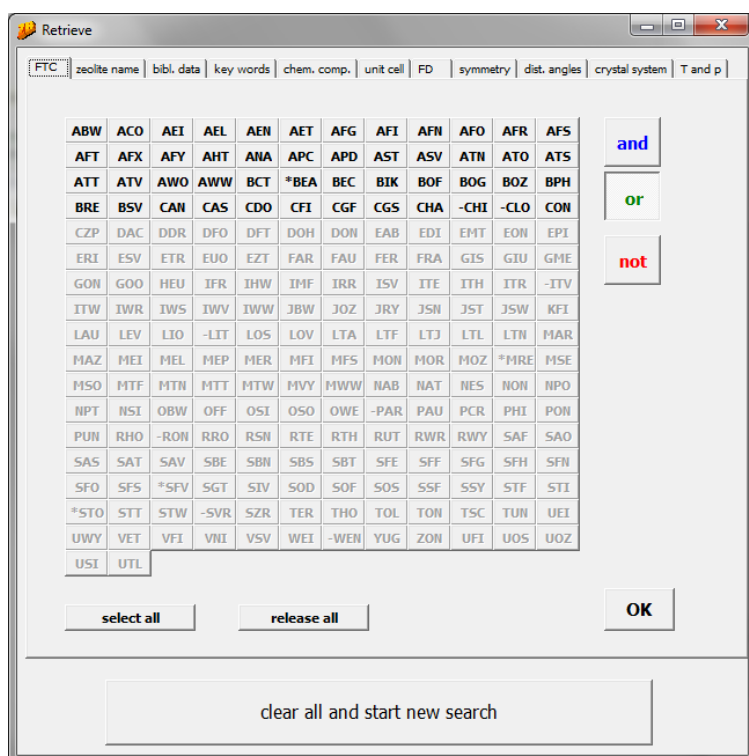


Fig. 3.2.2: Framework type code menu

This tab sheet contains buttons for all framework types (currently 206) accepted by the Structure Commission of the International Zeolite Association. However, the first releases and beta-versions of the database might be restricted to a subset of framework types. Accessible codes are labelled with black letters, nonaccessible codes are light grey. Note that Boolean operators "and" and "not" must be selected before pressing an FTC button to be applied. "or" is preselected by default. If "and" is selected as Boolean operator, only one FTC button can be pressed (one entry cannot belong to more than one code). Alternatively, the "select all" button can be pressed for selecting all entries (only for "or" operator). The "release all" button resets all buttons to unselected. The big button on the bottom ("clear all and start new search") applies to all retrieval menus and resets the whole retrieval session.

If the selection for all retrieval items is complete, press “OK” to continue. Do not press “OK” if further items in other tab sheets of the retrieval menu are to be selected. “OK” will terminate the retrieval and displays the results.

3.2.3 Zeolite Name

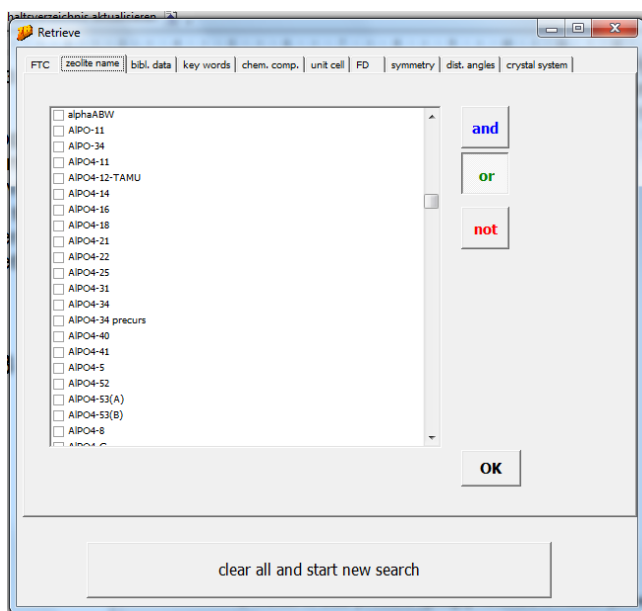


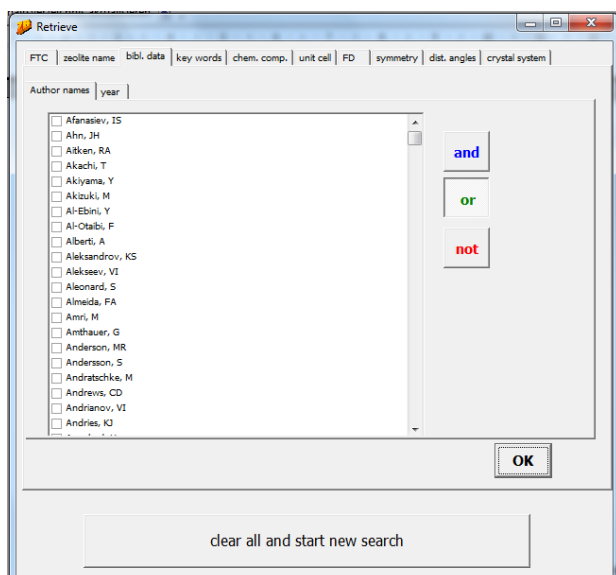
Fig. 3.2.3: Zeolite name menu

Zeolite names (mineral names, synthetic compound designations) are listed in alphabetical order. Items are selected by clicking in the respective checkbox. The color of the selected item will turn to the color of the Boolean operator. The item can be unselected by clicking again on the checkbox with the checkmark.

The big button on the bottom (“clear all and start new search”) applies to all retrieval menus and resets the whole retrieval session.

If the selection for all retrieval items is complete, press “OK” to continue. Do not press “OK” if further items in other tab sheets of the retrieval menu are to be selected. “OK” will terminate the retrieval and displays the results.

3.2.4 Bibliographic data



This tab sheet is divided into two sections: “Author names” and “year” of publication.

Author names are sorted in alphabetical order. The selection process is identical to the selection of zeolite names in 3.2.3.

If the selection for all retrieval items is complete, press “OK” to continue. Do not press “OK” if further items in other tab sheets of the retrieval menu are to be selected. “OK” will terminate the retrieval and displays the results.

Fig. 3.2.4: Author name menu



The year of publication or the respective period can be defined by entering the first and the last year within which the entries are to be selected. After pressing “select” the year or the period is entered into the grid. The number of periods consisting of first and last year is unlimited for “or” and “not” operators. That way, all publications between, e.g., 1970 and 1980, and between 2000 and 2010 can be selected. The same way, entries can be removed from the grid (and consequently from the retrieval) by pressing the “unselect” button.

Fig. 3.2.5: Year of publication menu

If the selection for all retrieval items is complete, press “OK” to continue. Do not press “OK” if further items in other tab sheets of the retrieval menu are to be selected. “OK” will terminate the retrieval and displays the results.

3.2.5 Keywords

Keywords are sorted in alphabetical order. The selection process is identical to the selection of zeolite names in 3.2.3. The following keywords are available

- “Powder diffraction, non-Rietveld”: All refinements against powder diffraction data except Rietveld-refinements
- “Rietveld refinement”
- “Single-crystal refinement”
- “Theoretical calculation”: Theoretical calculations of crystal structures except distance least squares refinements
- “X-ray diffraction”
- “Neutron diffraction”
- “Electron diffraction”
- “Synchrotron radiation”
- “Simulated structure”
- “Distance least squares refinement”
- “Combined neutron and X-ray diffraction”
- “Data incomplete”: Some data are missing in the entry which could not be supplied by us
- “Entry modified”: Data have been edited by us as documented in the remarks
- “Mineral”
- “Synthetic compound”
- “No thermal treatment”
- “Dehydrated”
- “Calcined”: Thermal treatment at temperatures causing severe changes in the crystal structure beyond dehydration
- “No chemical treatment”
- “Cation exchanged”
- “Acid treatment”
- “Phase transformation”
- “constrained refinement”

The selection process is identical to the selection of zeolite names in 3.2.3.

If the selection for all retrieval items is complete, press “OK” to continue. Do not press “OK” if further items in other tab sheets of the retrieval menu are to be selected. “OK” will terminate the retrieval and displays the results.

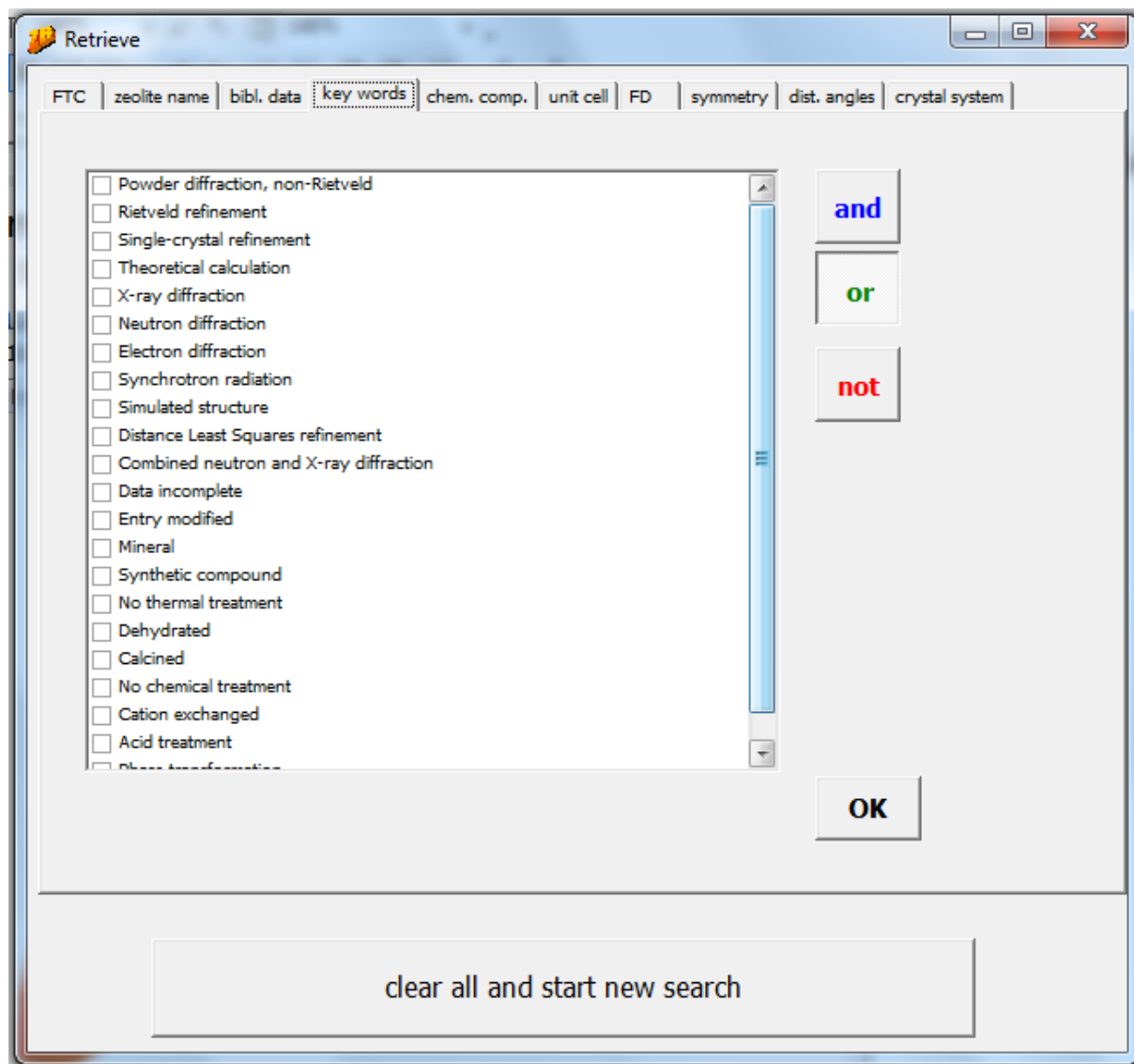


Fig. 3.2.6: Key word menu

3.2.6. Chemical composition

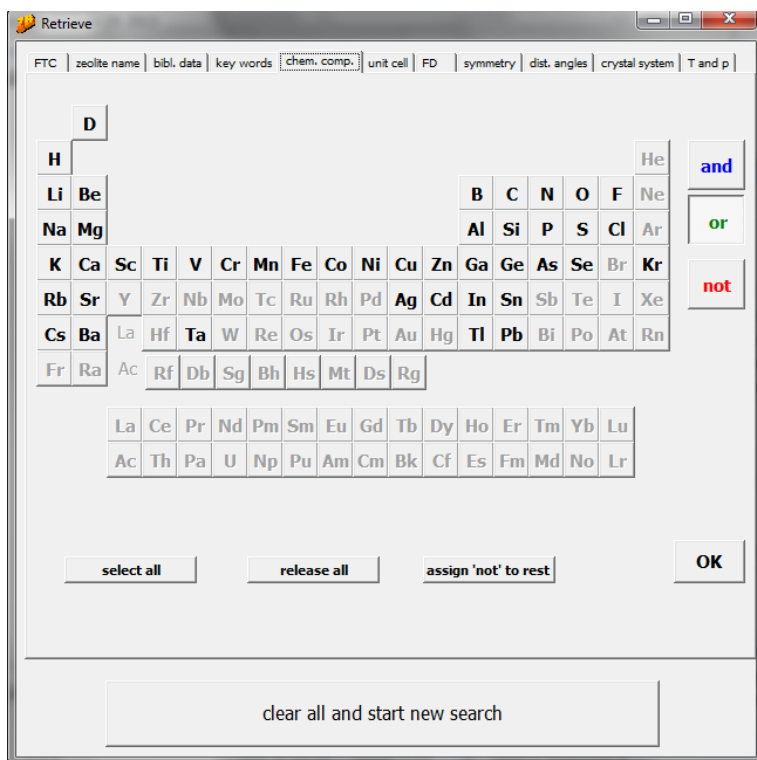
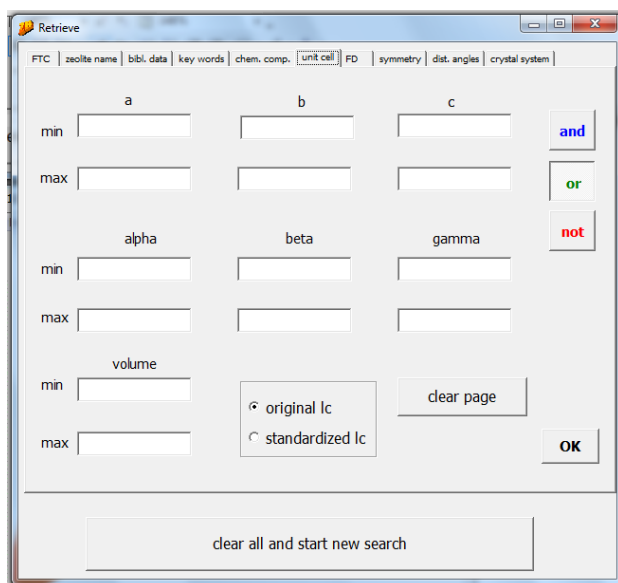


Fig. 3.2.7: Chemical composition menu

The chemical composition can be selected by pressing the respective element combined with a Boolean operator. Only those elements are highlighted in the periodic table of elements which are present in the entries of the database. The others are not activated. The “select all” button enables all highlighted elements and the “release all” button resets all elements. After selecting one or more elements with either “and” or “or” operator, the rest can be flagged as “not”, thus restricting the chemical composition to the selected elements.

If the selection for all retrieval items is complete, press “OK” to continue. Do not press “OK” if further items in other tab sheets of the retrieval menu are to be selected. “OK” will terminate the retrieval and displays the results.

3.2.7 Unit-cell parameters

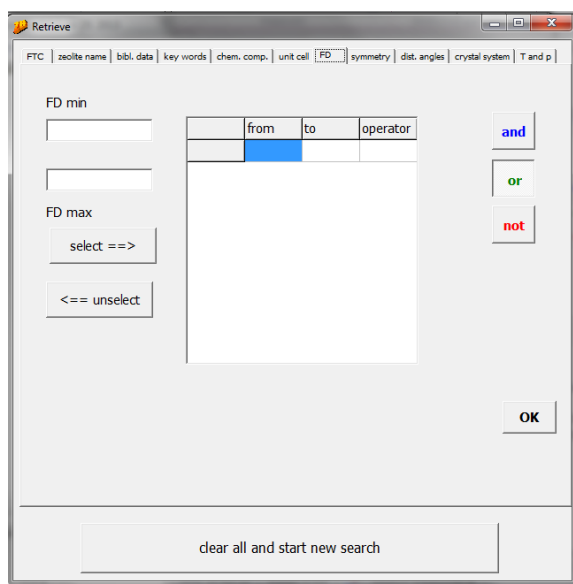


The range can be specified for all six unit-cell parameters and the unit-cell volume within the selected entries. The user can choose between the setting of the original work and the standardized setting of the unit cell. The “clear page” button resets all edit fields on this tab sheet.

If the selection for all retrieval items is complete, press “OK” to continue. Do not press “OK” if further items in other tab sheets of the retrieval menu are to be selected. “OK” will terminate the retrieval and displays the results.

Fig. 3.2.8: Unit cell parameter menu

3.2.8 Framework density



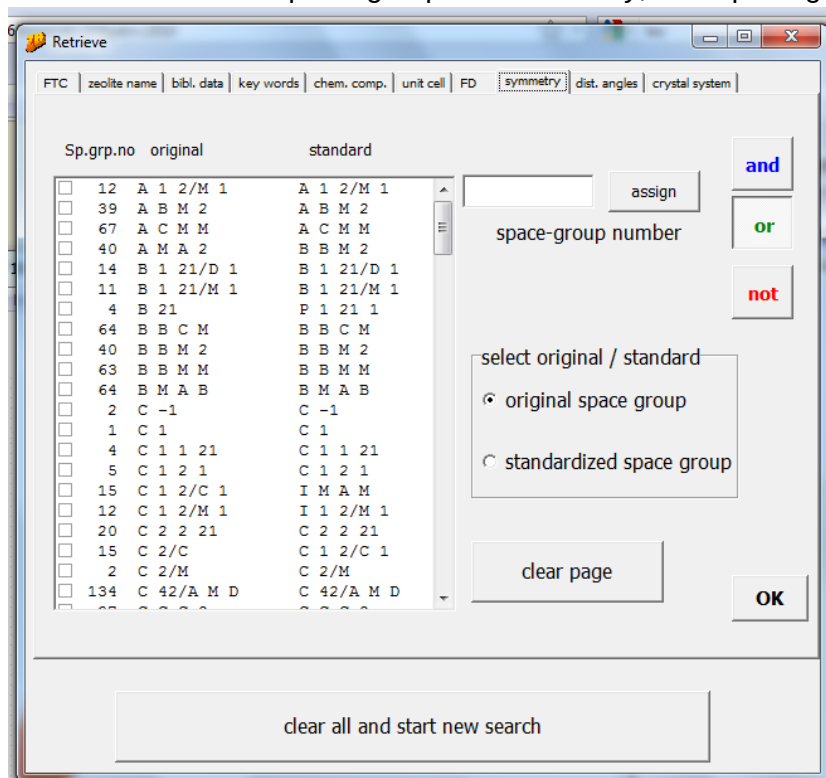
The range of the framework density can be defined by entering the minimum and maximum FD values within the entries. After pressing “select” the FD or the range of FD is entered into the grid. The number of FD data pairs is unlimited for “or” and “not” operators. That way, all FD ranges, e.g., between 10 and 12, and between 17 and 19 can be selected. The same way, entries can be removed from the grid (and consequently from the retrieval) by pressing the “unselect” button.

Fig. 3.2.9: Unit-cell parameter menu

If the selection for all retrieval items is complete, press “OK” to continue. Do not press “OK” if further items in other tab sheets of the retrieval menu are to be selected. “OK” will terminate the retrieval and displays the results.

3.2.9 Space-group symmetry

The selection is similar to the selection of zeolite names in 3.2.3. However, the user has the choice to select either space groups in the original settings or in the standardized settings. The selection cannot be mixed, i.e., just one of the two setting types can be applied to all items in the list of space groups. Alternatively, the space-group number can be entered



which is then assigned to all space groups with the same number irrespectively of their settings. Press “assign” after entering the number. The “clear page” button resets all space group selections.

If the selection for all retrieval items is complete, press “OK” to continue. Do not press “OK” if further items in other tab sheets of the retrieval menu are to be selected. “OK” will terminate the retrieval and displays the results.

Fig. 3.2.10: Symmetry menu

3.2.10 Distances and angles

Minimum and maximum values can be entered to specify the range for mean T-O distances, T-O-T angles, and O-T-O angles as well as for the corresponding errors and the mean deviation (designated sig(xyz)) of framework coordinates from the aristotype structure. The latter option gives a good measure for the mean deviation of the framework structure from the higher symmetry. The “clear page” button resets all edit fields in this tab sheet.

If the selection for all retrieval items is complete, press “OK” to continue. Do not press “OK” if further items in other tab sheets of the retrieval menu are to be selected. “OK” will terminate the retrieval and displays the results.

Fig. 3.2.11: Distances and angles menu

3.2.11 Crystal system

Fig. 3.2.12: Crystal systems menu

Crystal systems can be selected by clicking on the respective checkboxes or the corresponding text. Only one entry can be selected if the operator “and” is active. Note that there are three options for trigonal structures: (1) trigonal, selecting all but rhombohedral entries; (2) rhombohedral hexagonal setting, selecting all rhombohedral structures with hexagonal setting in the original entries; (3) rhombohedral primitive setting, selecting all rhombohedral structures with rhombohedral axes in the original entries. Thus, all structures with trigonal space groups including rhombohedral are selected by checking all three items, all rhombohedral structures are selected by checking the two rhombohedral items.

If the selection for all retrieval items is complete, press “OK” to continue. Do not press “OK” if further items in other tab sheets of the retrieval menu are to be selected. “OK” will terminate the retrieval and displays the results.

3.3 List of selections

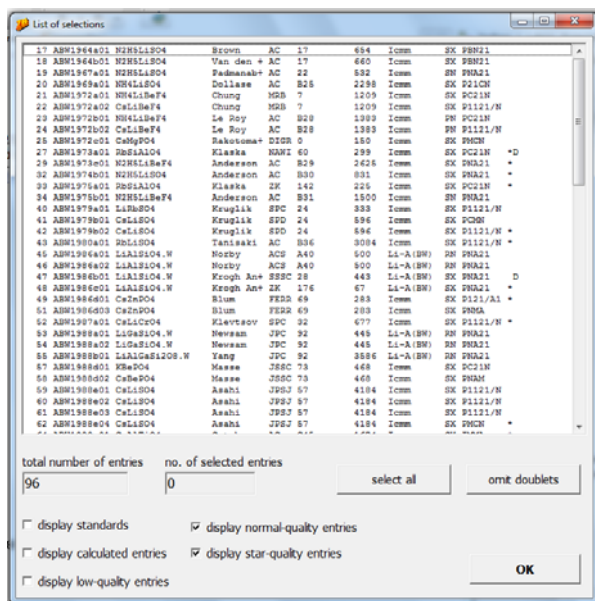


Fig. 3.3.1: List of selections

After finishing the retrieval by pressing OK on one of the retrieve tab sheets, the list of selected items appears in a separate window. Fig. 3.3.1 shows the list of selections after selecting ABW in the FTC retrieval menu. By default all normal-quality and star-quality entries are displayed. Standard entries and low-quality entries can be added to the list by checking the respective checkboxes.

The selection of entries from this list works as in standard windows selections.

Single entry: Click on respective entry

Consecutive entries: Click on first entry, press shift and click on last entry.

Various entries: Press the cntl key and click on all entries to be selected.

With the “select all” button all entries are selected.

Doublets (entries essentially identical to other entries) can be omitted by pressing the “omit doublets” button.

The total number of entries listed and the number of entries selected are given in the two frames underneath the list.

Press “OK” to continue after selection is complete.

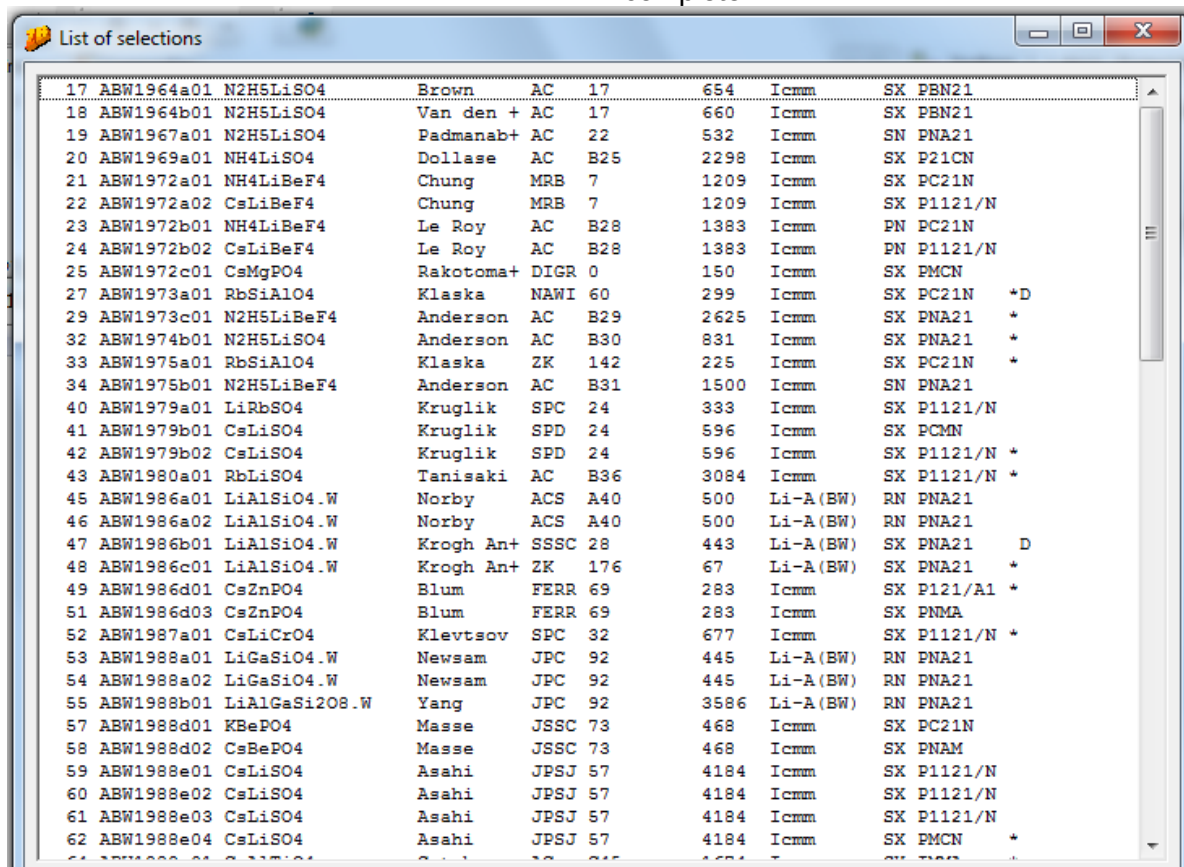


Fig. 3.3.2 List of selections, enlarged.

A single line (entry) contains the following information from left to right

- Sequence number of entry, reassigned in every new release of ZeoBase
- Unique code for a single entry preserved in all versions of ZeoBase, consisting of the FTC, year of publication, letter assigned to the publication, number assigned to the crystal structure data set in a specific publication
- Short form of approximate chemical composition
- Last name of first author
- Journal code (see chapter 5.1)
- Volume number
- Number of first page
- Sample designation, mineral name, or group names
- Capital letter for analysis method (P: powder diffraction, non-Rietveld; R: Rietveld refinement; S: Single-crystal structure refinement; T: theoretical calculation; M: modelled structure, usually combined with powder-pattern simulation)
- Capital letter for method of data collection (X: X-rays; N: neutrons; E: electrons; Y: synchrotron; S: simulated; D: DLS calculation; B: joint neutron and X-ray)
- Space-group symbol

Flags in last column

- \$ Standard entry¹⁾
- * High-quality entry²⁾
- Low-quality entry³⁾
- D Doublet⁴⁾

blank Normal entry⁵⁾

1) Entry used for standardization of entries of a given FTC in a specific space group.

2) Entries with $\text{esd}(\text{T-O})_{\text{mean}} < 0.01 \text{ \AA}$, and $\text{DI}(\text{TO}) > 0.03$.

3) Entries containing obvious errors which could not be fixed, or entries without esd values for the positional coordinates, or entries with extremely large deviations from expected bond lengths or angles or entries with huge esd-values of their bond lengths.

4) Entry published two or three times by the original authors. The first occurrence is not marked by a D, the following ones are.

5) All entries not belonging to the above categories.

The reasons for the classifications are explained in the comments accessed in Edit/view.

3.4 Edit/view menu

3.4.1 Overview

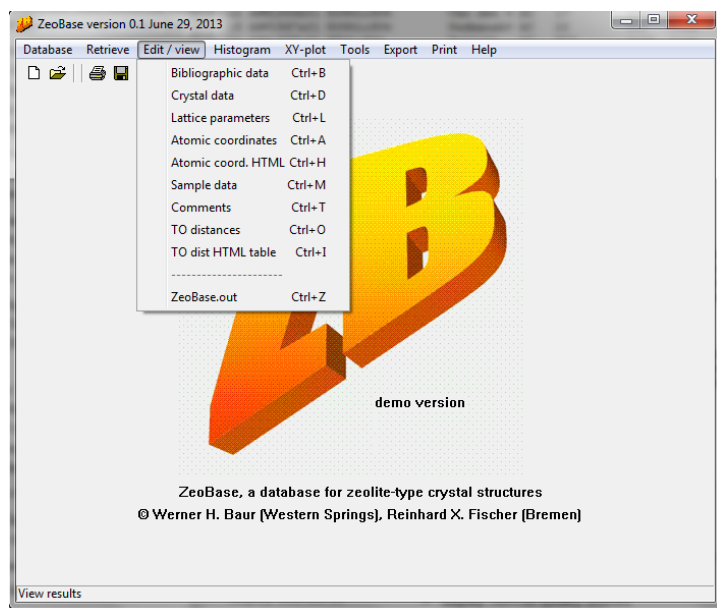


Fig. 3.4.1: Edit/view pulldown menu

The edit/view menu displays the results of the retrieval and the zeobase.out file where various information on the current session is recorded, dependent on the last action. Every item in this menu can be accessed by hotkeys displayed in Fig. 3.4.1.

If more than one entry is selected in the retrieval process, the output information is written consecutively for each entry.

3.4.2 Bibliographic data

Full reference is given for all entries selected in the list of selections (chapter 3.3). For printing contents of frame see chapter 3.9

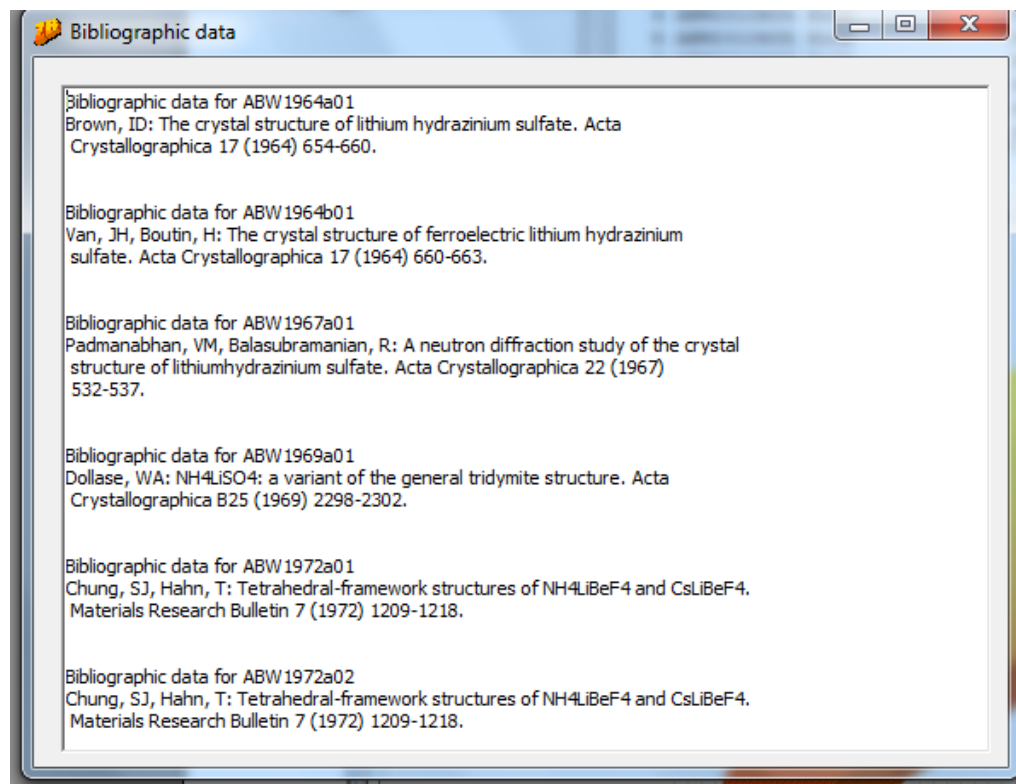
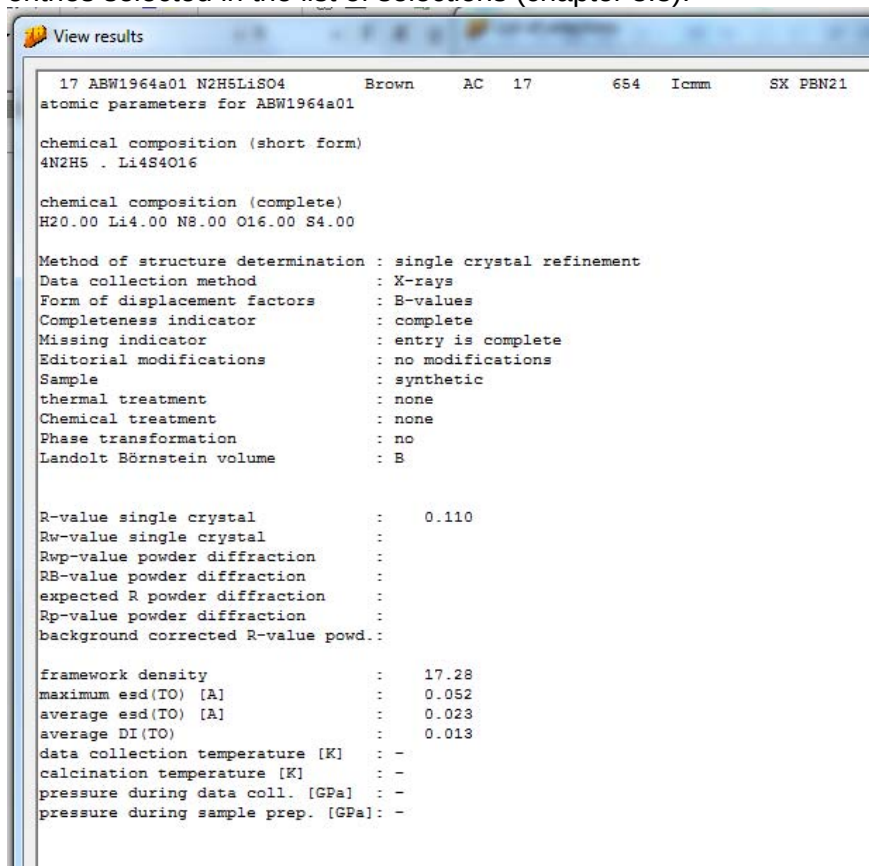


Fig. 3.4.2: Full References for selected entries

3.4.3 Crystal data

Crystal data (including general information on entries, chemical composition, space group, lattice parameters, atomic parameters, residuals) are listed in consecutive order for all entries selected in the list of selections (chapter 3.3).



View results

17 ABW1964a01 N2H5LiSO4 Brown AC 17 654 Icmm SX PBN21

atomic parameters for ABW1964a01

chemical composition (short form)
4N2H5 . Li4S4O16

chemical composition (complete)
H20.00 Li4.00 N8.00 O16.00 S4.00

Method of structure determination : single crystal refinement

Data collection method : X-rays

Form of displacement factors : B-values

Completeness indicator : complete

Missing indicator : entry is complete

Editorial modifications : no modifications

Sample : synthetic

thermal treatment : none

Chemical treatment : none

Phase transformation : no

Landolt Börnstein volume : B

R-value single crystal : 0.110

Rw-value single crystal : 0.052

Rwp-value powder diffraction : 0.023

RB-value powder diffraction : 0.013

expected R powder diffraction : 0.013

Rp-value powder diffraction : 0.013

background corrected R-value powd.: 0.013

framework density : 17.28

maximum esd(TO) [Å] : 0.052

average esd(TO) [Å] : 0.023

average DI(TO) : 0.013

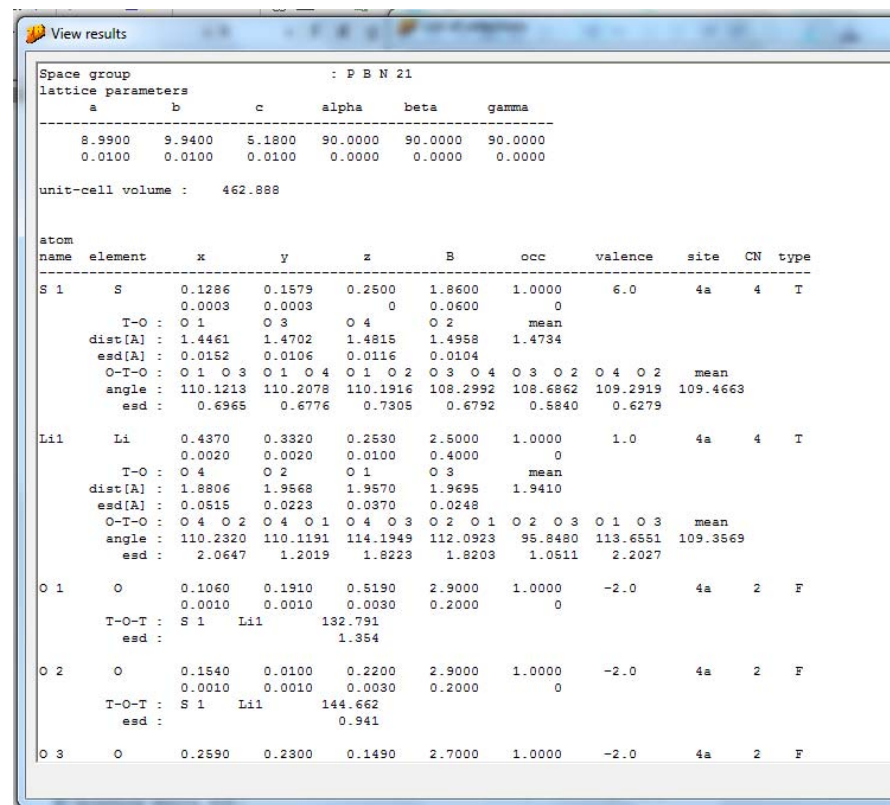
data collection temperature [K] : -

calcination temperature [K] : -

pressure during data coll. [GPa] : -

pressure during sample prep. [GPa] : -

Fig. 3.4.3: First part of crystal data with chemical composition, information on entry, residuals, framework density, space group, and lattice parameters.



View results

Space group : PBN 21

Lattice parameters

a	b	c	alpha	beta	gamma
8.9900	9.9400	5.1800	90.0000	90.0000	90.0000
0.0100	0.0100	0.0100	0.0000	0.0000	0.0000

unit-cell volume : 462.888

atom

name	element	x	y	z	B	occ	valence	site	CN	type
S 1	S	0.1286	0.1579	0.2500	1.8600	1.0000	6.0	4a	4	T
	T-O	0.0003	0.0003	0	0.0600	0				
	dist[Å]	1.4461	1.4702	1.4815	1.4958	1.4734				
	esd[Å]	0.0152	0.0106	0.0116	0.0104					
	O-T-O	0.1 0.3	0.1 0.4	0.1 0.2	0.3 0.4	0.3 0.2	0.4 0.2	mean		
	angle	110.1213	110.2078	110.1916	108.2992	108.6862	109.2919	109.4663		
	esd	0.6965	0.6776	0.7305	0.6792	0.5840	0.6279			
Li1	Li	0.4370	0.3320	0.2530	2.5000	1.0000	1.0	4a	4	T
	T-O	0.0020	0.0020	0.0100	0.4000	0				
	dist[Å]	1.8806	1.9568	1.9570	1.9695	1.9410				
	esd[Å]	0.0515	0.0223	0.0370	0.0248					
	O-T-O	0.4 0.2	0.4 0.1	0.4 0.3	0.2 0.1	0.2 0.3	0.1 0.3	mean		
	angle	110.2320	110.1191	114.1949	112.0923	95.8480	113.6551	109.3569		
	esd	2.0647	1.2019	1.8223	1.8203	1.0511	2.2027			
O 1	O	0.1060	0.1910	0.5190	2.9000	1.0000	-2.0	4a	2	F
	T-O-T	S 1	Li1	132.791	0.2000	0				
	esd			1.354						
O 2	O	0.1540	0.0100	0.2200	2.9000	1.0000	-2.0	4a	2	F
	T-O-T	S 1	Li1	144.662	0.2000	0				
	esd			0.941						
O 3	O	0.2590	0.2300	0.1490	2.7000	1.0000	-2.0	4a	2	F

Fig. 3.4.4: Second part of crystal data with atomic parameters (atom name, chemical element, coordinates x,y,z, isotropic displacement parameter B, site occupancy factor, valence, Wyckoff site symbol, coordination number CN, type of atom: T = tetrahedrally coordinated framework atom, F = framework anion) T-O distances for framework atoms with standard deviations, O-T-O and T-O-T angles of framework atoms.

	min	max
T-O mean [Å]	1.473	1.941
sig(T-O) mean [Å]	0.012	0.034
T-O-T angle [°]	132.791	144.662
sig(T-O-T angle) [°]	0.641	1.460
O-T-O angle [°]	95.848	114.195
sig(O-T-O angle) [°]	0.404	0.702
mean sig(xyz)	0.000	0.010
mean deviation from standard [Å]:	0.474	

Fig. 3.4.5: Last part of crystal data with statistical information on minimum and maximum values for distances and angles. The last number represents the mean deviation of all coordinates from the aristotypic structure.

3.4.4 Lattice parameters, Atomic coordinates, Atomic coord. HTML, Sample data, Comments, TO distances, TO dist HTML table

These menu items list the respective parameters separately for better comparison. For a full set with all information select crystal data. Atomic coordinates and T-O distances can be listed in a HTML formatted table. These tables can be imported in any HTML compatible word processing system like, e.g., Microsoft Word. However, some versions of Word display horizontal lines as thick bars which can be deleted by hand and replaced with normal lines. If the HTML frame is the active window it can be saved using the save active frame option in pull down menu Export (see chapter 3.8.4).

3.4.5 Zeobase.out, zeograph.out

This option lists the zeobase.out file written by various parts of ZeoBase. Especially data used for the histograms and XY-plots are written to zeobase.out. If the zeobase.out frame is the active window it can be saved using the save active frame option in pull down menu Export (see chapter 3.8.4). Similarly, it can be printed using the print option in the main menu (see chapter 3.9).

3.5 Histograms

After selecting one or more entries in the list of selections, histograms displaying the frequency of occurrences of various parameters can be drawn. The respective items to be displayed can be selected on six tabsheets with lattice parameters, framework contents, distances, angles, distortion indices, and temperatures. Dependent on the choice of parameters, edit frames may appear or disappear on the tabsheets which allow to specify individual parameters. That way, e.g., T-O distances can be listed for specific T and/or O atoms. Wildcards can be entered as an asterisk. Fig. 3.5.1 shows, e.g., the distances tabsheet where the T-O individual button is selected. Eight edit fields appear, four for the T-atom and another four for the O-atom, where the individual atoms can be specified. Leaving the wildcards (*) as default setting in the fields yields all mean distances of all TO4 tetrahedra irrespectively of any atom specifications. If the user wants to have SiO distances only, then Si and O should be entered as atom names. This could be further reduced to list distances between Si1 and O2; then 1 should be entered in the second field after Si and 2 should be entered in the second field after O. This will yield all distances between Si1** and O2** where the asterisks stand for any number or letter. Instead, Si 1 1 a and O 2 1 b could be entered to list Si11a-O21b distances only. The unit (Å, nm, pm) can be selected by clicking on the

respective radio buttons. The selection of entries can be limited to those with fully occupied T positions by clicking on the respective check box.

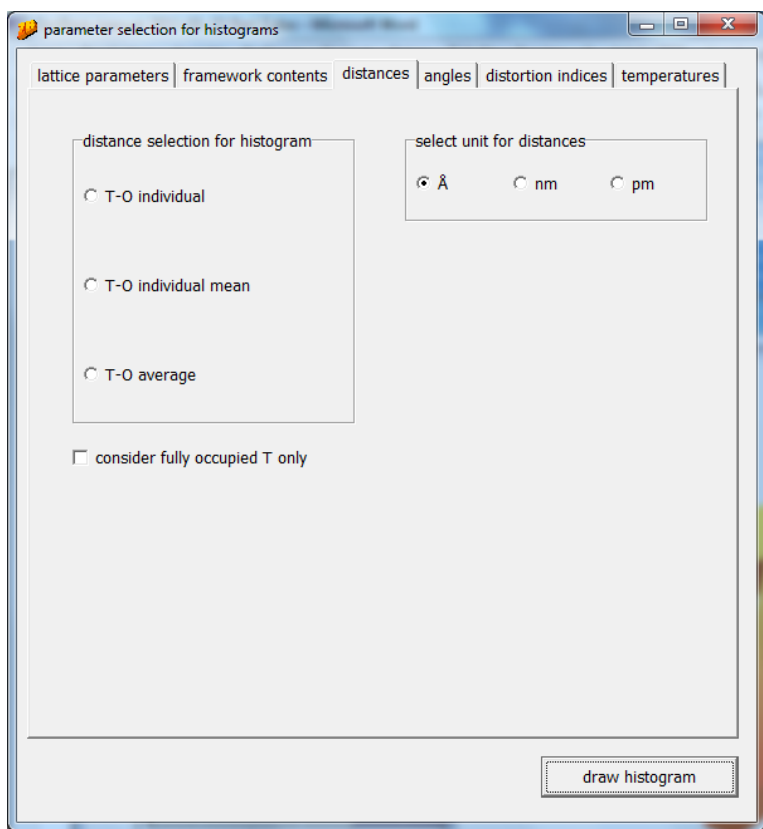


Fig. 3.5.1 Distances tabsheet

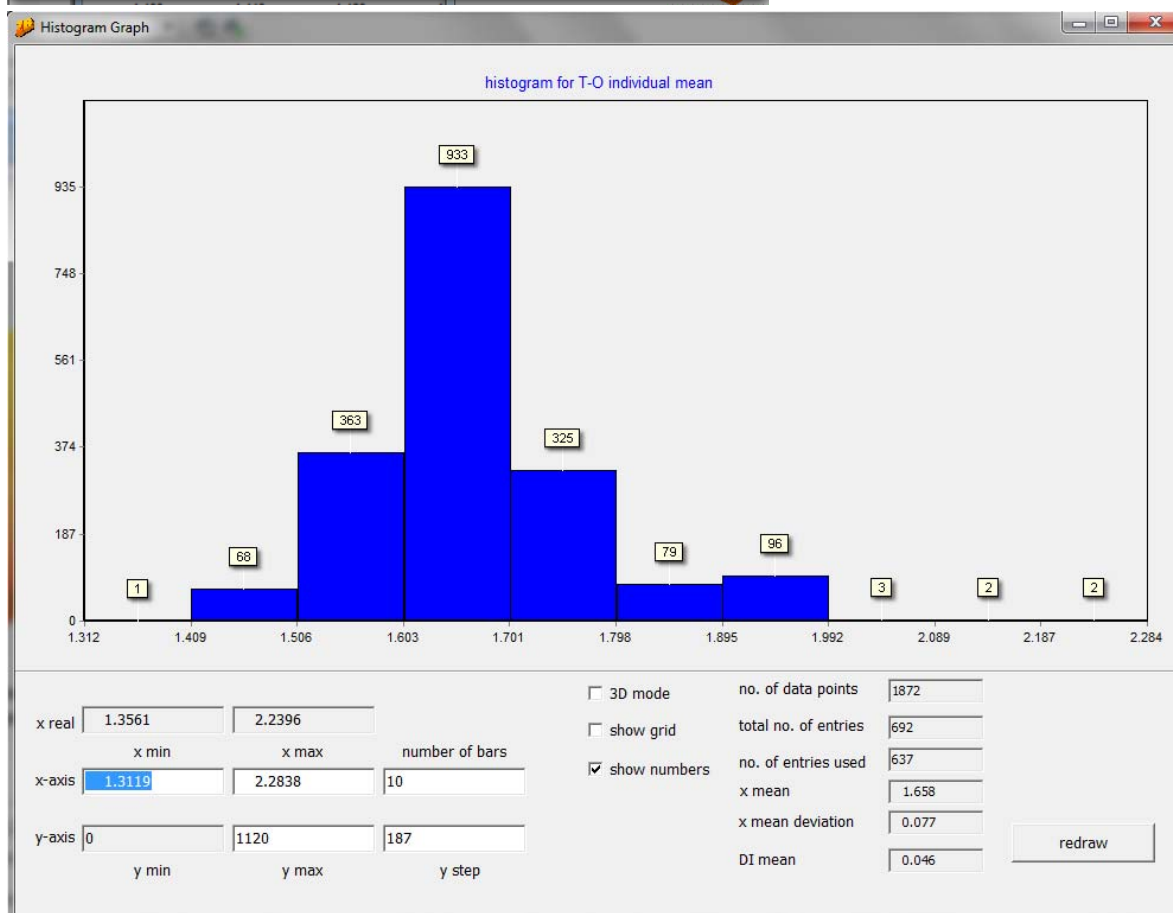


Fig. 3.5.2 Histogram of mean T-O distances in ANA type compounds.

After selecting the respective item to be listed, the histogram will be drawn with default settings listed in the edit fields below the histogram. These parameters can be edited as done in Fig. 3.5.2 for a plot of mean T-O distances in ANA type compounds (normal and star-quality entries only). Noneditable parameters are in grey fields. If the histogram frame containing the graphical display is the active window it can be printed using the print option in the main menu (see chapter 3.9).

3.6 XY-plots

XY-plots are done in a similar way as histograms. Two panels with various tabsheets will appear as shown in Fig. 3.6.1: The left one for the selection of parameters to be plotted on the ordinate, the right one for the abscissa. As in the case of histograms, edit fields are available for individual parameters to specify the designations of the involved atoms. In the example in Fig. 3.6.1, where individual T-O-T angles are to be plotted versus the framework density, atom names can be specified for the two T-atoms and the bridging O-atom (here, they are left on the default setting with an asterisk in all fields as wild-card for any atom).

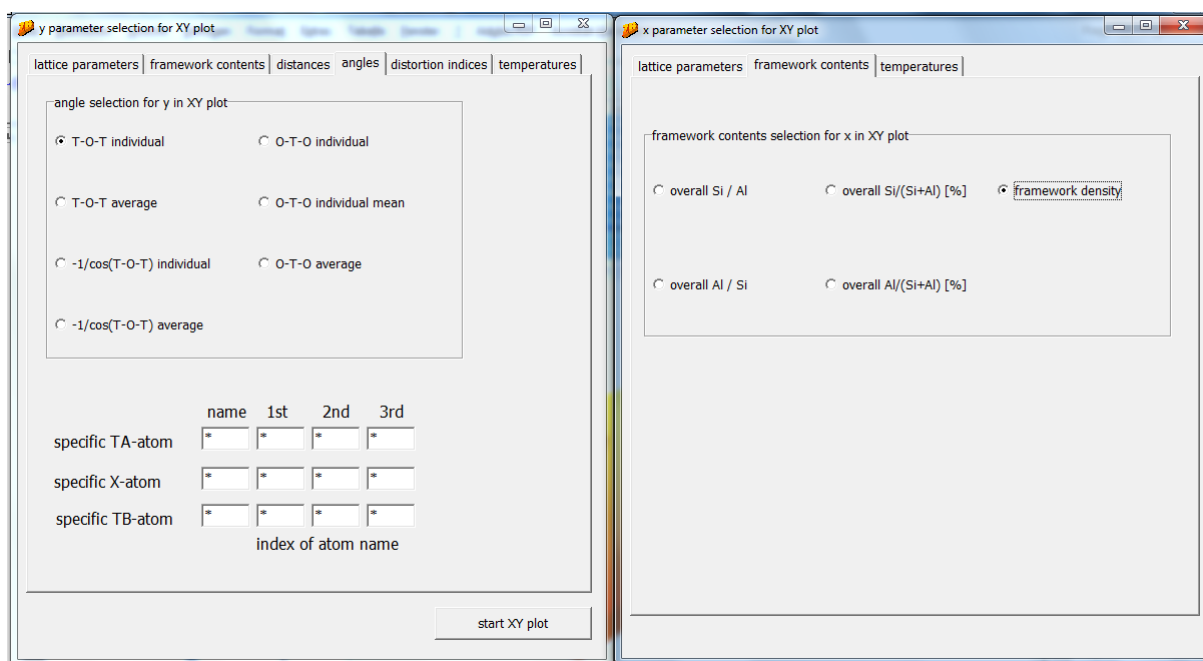


Fig. 3.6.1 Tabsheet for the selection of parameters to plotted in the XY-diagram

After selecting the parameters in the two panels, press “start XY plot”. The XY-plot will appear in the upper frame as shown in Fig. 3.6.2 with default values for the X and Y axes. These settings can be changed in the edit fields below the plot and pressing the “redraw” button. A grid with horizontal and vertical lines can be added by clicking in the checkbox “show grid”. A regression line according to $Y=a_0+a_1x+a_2x^2+a_3x^3+\dots+a_{10}x^{10}$ can be calculated after selecting the respective degree of polynomial. The regression curve will be plotted and the least squares parameters are shown in the output frame. Definitions are:

$$\chi^2 = \sum_i (y_{io} - y_{ic})^2, \text{ goodness of fit: } GOF = \frac{\sum_i (y_{ic} - \bar{y}_c)^2}{\sum_i (y_{io} - \bar{y}_o)^2}, \text{ residual: } R = \frac{\sum_i |y_{io} - y_{ic}|}{\sum_i |y_{io}|}$$

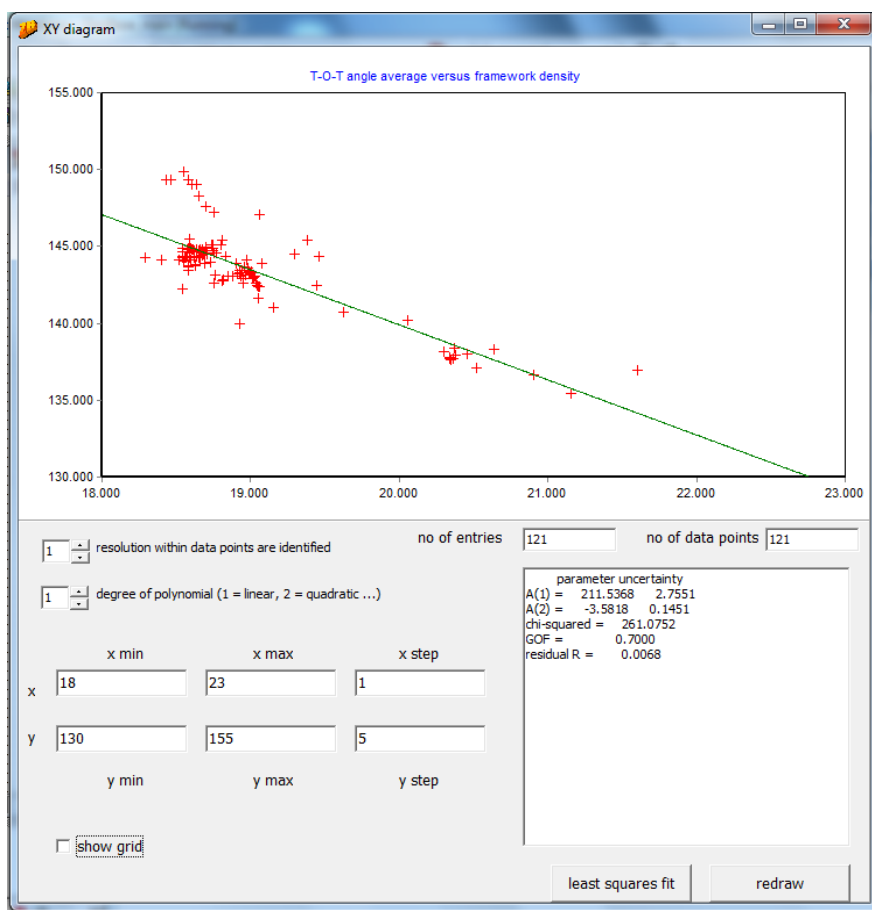


Fig. 3.6.2: XY-plot of T-O-T angles versus framework density of ANA type aluminosilicates, with the green line representing the linear regression.

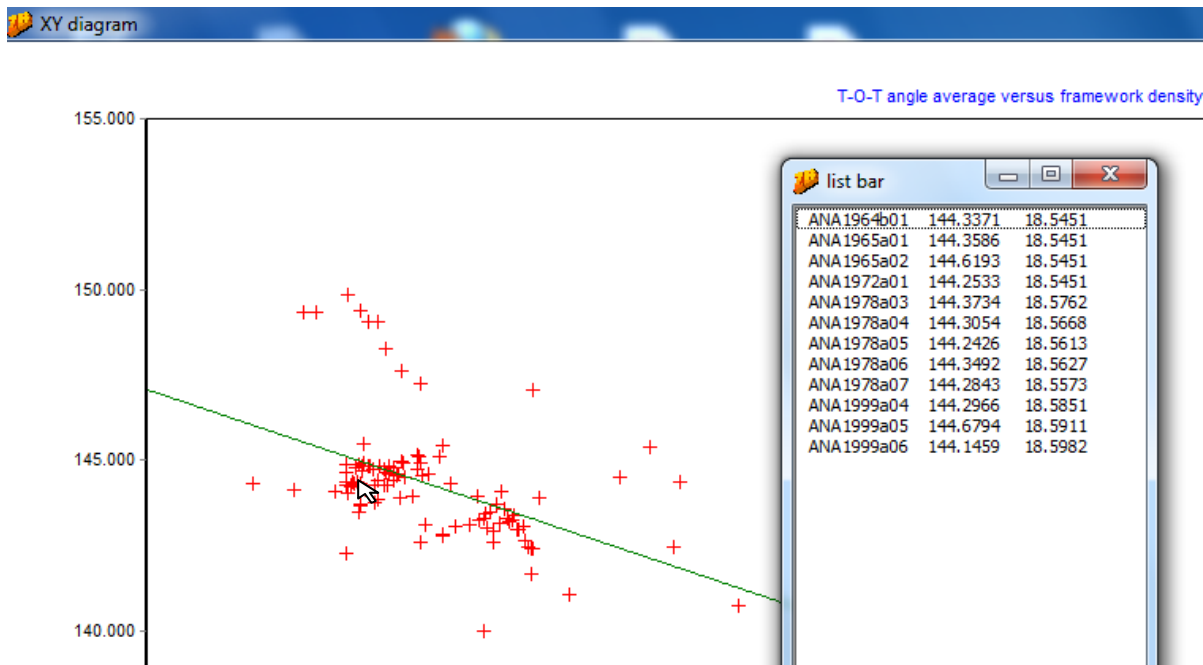


Fig. 3.6.3: Identification of data points.

After the XY plot is displayed data points can be identified by right click on the red crosses. All entries are displayed in the list bar which lie within a certain resolution (pixels) around the cursor position. This resolution can be defined by clicking on the up-down buttons underneath the graphics display.

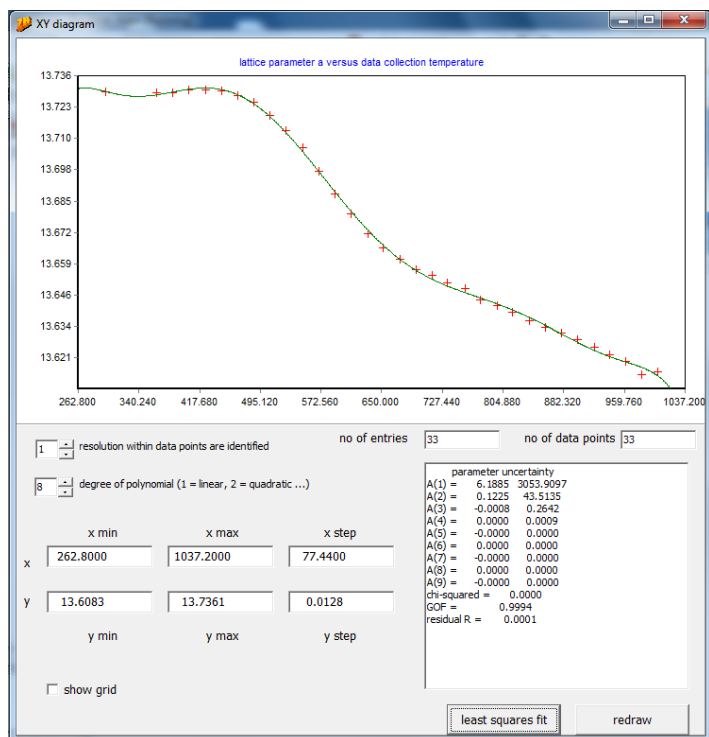


Fig. 3.6.4: XY-plot (default plot, axes parameters not edited) of lattice parameter a versus data-collection temperature for ANA1999a entries with the green curve representing the 8th degree fit.

3.7 Tools

3.7.1 Distances and angles

A table of distances and angles is generated for the selected entries. Estimated standard deviations can be listed as numbers behind or below the respective values or they can be listed in parentheses after the last significant digit. Numbers in the first column of atom names refer to the list of generated atom positions which can be listed on clicking on the checkbox "Display list of atoms" and then pressing the calc button. Minimum and maximum values within distances are listed can be specified in the edit fields.

3.7.2 SADIAN

Alternatively to 3.7.1, distances and angles can be calculated using the program SADIAN [10]. A detailed description to use SADIAN as standalone program will be provided soon. Here, it is started automatically with default values and the results are displayed which can be stored or printed.

3.7.3 STRUPLO

A structure drawing can be generated using STRUPLO [11]. By default, atoms are drawn as spheres without any bonds.

A detailed description will be provided soon. Here, it is started automatically with default values and the results are displayed which can be stored or printed using the internal options in STRUPLO.

3.7.4 Powder pattern

A powder pattern is simulated using the Rietveld program BRASS [12]. A detailed description will be provided soon.

3.7.5 BRASS

Full access to the Rietveld program BRASS [12] is available.
A detailed description will be provided soon.

3.8 *Export*

3.8.1 cif

Space group symbol, lattice parameters, and atomic coordinates are written on zeobase.cif in cif format.

3.8.2 SADIAN

An input file for the distance and angle program SADIAN [10] is written on sad.inp. Note that distances and angles can be calculated directly by selecting SADIAN in the tools menu.

3.8.3 STRUPLO

An input file for the old DOS version of STRUPLO is written on struplo.str. This file can be read by the windows version as well. Note that a STRUPLO plot can be generated directly by selecting STRUPLO in the tools menu.

3.8.4 Save active frame

Most of the output displayed in separate frames can be saved using this option. The user will be prompted for directory and file names. The last active frame will be saved always. Alternatively, the short cut cntl+s can be used on main menu level. In the demo version, saving is only possible by selecting the icons on the main frame (Fig. 3.1.1) or using the above mentioned shortcuts if the main frame is the active frame.

3.9 *Print*

This option will print the contents of output frames. The last active frame will be printed always. The user will be prompted to select printer and print options. The short cut cntl+p can be used on main menu level. Alternatively, the text to be printed can be marked and transferred by copy (Ctrl+C) and paste (Ctrl+V) to a windows compatible word or text processing system. In the demo version, printing is only possible by selecting the icons on the main frame (Fig. 3.1.1) or using the above mentioned shortcuts if the main frame is the active frame.

3.10 *Help*

This option is not available yet

4. References

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- [8] Kahlenberg, V, Fischer, R.X. & Baur, W.H.: Z. Krist. **216** (2001) 489-494.
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- [10] Baur, W.H., Kassner, D., Z. Kristallogr. Suppl. **3** (1991) 15.
- [11] Fischer, R.X., Messner, T.: STRUPLO. Universität Bremen 2013
- [12] Birkenstock, J, Messner, T., Fischer, R.X.: BRASS, the Bremen Rietveld Analysis and Structure Suite. Universität Bremen 2013, www.brass.uni-bremen.de

5. Appendix

5.1 *Journal codes*

In some menus and output frames (see, e.g., chapter 4) 2-4 letter codes are used for the abbreviation of journals, books, theses, and electronic media. The following is a complete list with all abbreviations.

AANL	Atti della Accademia Nazionale dei Lincei, Classe di Scienze Fisiche+, Rendiconti, S. 8
AAST	Atti della Accademia delle Scienze di Torino
AAWM	Anzeiger der Oesterreichischen Akademie der Wissenschaften, Math-Naturw. Kl
AC	Acta Crystallographica
ACAG	Applied Catalysis A: General
ACAP	American Crystallographic Association, Program and Abstracts
ACHS	Acta Chimica Sinica
ACS	Acta Chemica Scandinavica
ACSL	Acta Chimica Slovenica
ACSN	ACS Nano
ACSS	American Chemical Society, Symposium Series
ADCS	Advances in Chemistry Series
ADF	Anales de Fisica
ADM	Advanced Materials
AFQ	Anales de Fisica y Quimica
AGKG	Asahi Garasu Kogyo Gijutsu Shoreikei Kenkyu Hokoku
AGS	Acta Geologica Sinica
AICJ	American Institute of Chemical Engineers, Journal
AJC	Asian Journal of Chemistry
AKZ	Azerbaidzhan Khimia Zhurnal
AM	American Mineralogist
AMCS	Acta Montana
ANCH	Angewandte Chemie
ANCI	Angewandte Chemie, International Edition in English
AQUA	Anales de Quimica, Serie A, quimica fisica y quimica tecnica
AQIE	Anales de Quimica, International Edition
ASTS	Atti della Societa Toscana di Scienze Naturali residente in Pisa
ASXS	Analytical Sciences. X-ray Structure Analysis Online
AXCJ	Advances in X-ray Chemical Analysis Japan (X-sen Bunseki no Shinpo)
AXRA	Advances in X-Ray Analysis
BASC	Bulletin of the Academy of Sciences of the USSR Division Chemical Sciences
BBGP	Berichte der Bunsen-Gesellschaft-Physical Chemistry Chemical Physics
BCC	Bulgarian Chemical Communications
BCSJ	Bulletin of the Chemical Society of Japan
BK	Bunseki Kagaku- Japan Society for Analytical Chemistry
BKCS	Bulletin of the Korean Chemical Society
BM	Bulletin de Mineralogie
BSFM	Bulletin de la Societe Francaise de Mineralogie
CATL	Catalysis Letters
CATT	Catalysis Today
CC	Chemical Communications
CCCC	Collection of Czechoslovak Chemical Communications
CCL	Chinese Chemical Letters
CEJ	Chemistry, a European Journal
CGD	Crystal Growth & Design
CHEM	Chemistry of Materials
CHRV	Chemical Reviews
CI	Chemical Industries, Marcel Dekker, New York
CIGL	Carnegie Institution of Washington, Annual Report of the Director, Geophysical Laboratory
CJC	Chinese Journal of Chemistry
CJCT	Chinese Journal of Catalysis

CJCU	Chemical Journal of Chinese Universities
CJP	Canadian Journal of Physics
CLAM	Clay Minerals
CM	Canadian Mineralogist
CMGP	Centralblatt fur Mineralogie, Geologie und Palaontologie, Abteilung A.
CPL	Chemical Physics Letters
CR	Crystallography Reports
CRAB	Comptes rendus de l'Academie bulgare des Sciences
CRAS	Comptes Rendus Academie Sciences Paris
CRAC	Comptes Rendus Academie Sciences Paris, Serie II-Chimie
CRC	Comptes Rendus Chimie
CREN	Crystal Engineering
CRRV	Crystallography Reviews
CRT	Crystal Research and Technology
CS	Chemical Science
CSC	Crystal Structure Communications
CSP3	Collection of Simulated Powder Patterns, 3rd ed, 1996
CSPW	Collection of Simulated Powder Patterns, 5th ed, 2007, Website: http://www.iza-structure.org/databases
CX	Cuihua Xuebao, Dalian (Journal of Catalysis)
DAN	Doklady Akademii Nauk
DANE	Doklady of the Academy of Sciences of the USSR, Earth Science Sections
DCHE	Doklady Chemistry
DES	Doklady Earth Sciences
DGK	Deutsche Gesellschaft fur Kristallographie
DIBC	Dissertation University of British Columbia, Vancouver
DIBE	Dissertation Bern
DIBO	Dissertation Bochum
DICA	Dissertation Cambridge
DIDA	Dissertation Darmstadt
DIET	Dissertation ETH Zurich
DIFR	Dissertation Frankfurt
DIGE	Dissertation Geneva
DIGR	Dissertation Grenoble
DIHA	Dissertation Hannover
DIHH	Dissertation Hamburg
DIKI	Dissertation Kiel
DILE	Dissertation Katholieke Universiteit Leuven
DIMA	Dissertation Mainz
DIMC	Dissertation McMaster University
DIMR	Dissertation Marburg
DIPM	Dissertation Pierre et Marie Curie
DIPS	Dissertation Pennsylvania State University
DISB	Dissertation University of California, Santa Barbara
DIST	Dissertation Stockholm
DIWA	Dissertation University of Washington
DIWU	Dissertation Wurzburg
DPFR	Diplomarbeit Frankfurt
DPKI	Diplomarbeit Kiel
DT	Dalton Transactions
DZS	database of zeolite structures http://www.iza-structure.org/databases
DZT9	9. Deutsche Zeolith-Tagung, 3-5. Marz, 1997
EJIC	European Journal of Inorganic Chemistry
EJM	European Journal of Mineralogy
EJOC	E-Journal of Chemistry
EJSS	European Journal of Solid State and Inorganic Chemistry
EXPE	Experientia
FCMC	Fenzi Cuihua (J. Molecular Catalysis-Lanzhou-Chinese Edition)
FERR	Ferroelectrics
FM	Fortschritte der Mineralogie
FMB1	Fortschritte der Mineralogie, Beiheft 1
GCA	Geochimica and Cosmochimica Acta

GDFS	General Discussion of the Faraday Society, 1929
GEOK	Geokhimiya
GEOI	Geochemistry International, translation of Soviet journal Geokhimiya
GFBL	George Fisher Baker Lectureship at Cornell, F. M. Jaeger, MvGraw-Hill, 1930
GOOD	Geology of Ore Deposits
GPC	Glass Physics and Chemistry
GST	Proceedings of the International Symposium on Gas Separation Technology
GXXH	Gaodeng Xuexiao Huaxue Xuebao (Chemical J. of Chinese Universities)
HAHA	Habilitationsschrift Hannover
HAWU	Habilitationsschrift Wurzburg
HCA	Helvetica Chimica Acta
HRAT	Hydrothermal Reactions and Techniques, World Scientific, 2003
IC	Inorganic Chemistry
ICA	Inorganica Chimica Acta
ICC	Inorganic Chemistry Communications
ICSD	Inorganic Crystal Structure Database
IECR	Industrial & Engineering Chemistry Research
IJCA	Indian Journal of Chemistry, Section A, Inorganic, Bio-Inorganic, Physical
IJIM	International Journal of Inorganic Materials
IJP	Indian Journal of Physics
IM	Indian Mineralogist
IPPR	Intense Pulsed Neutron Source, Progress Report
IPSC	Italian Physical Society, Conference Proceedings
IZAW	Internat. Zeolite Assoc. Website, http://www.iza-structure.org/databases/
JAC	Journal of Applied Crystallography
JACO	Journal of Alloys and Compounds
JACR	Journal of the American Ceramic Society
JACS	Journal of the American Chemical Society
JAPP	Journal of Applied Physics
JC	Journal of Catalysis
JCAJ	Journal of the Ceramic Association of Japan
JCC	Journal of Chemical Crystallography
JCCH	Journal of Computational Chemistry
JCF1	Journal of the Chemical Society, Faraday Transactions I
JCIP	Journal de Chimie physique
JCIS	Journal of Colloid and Interface Science
JCP	Journal of Chemical Physics
JCRS	Journal of Chemical Research, Synapses
JCS	Journal of the Chemical Society
JCSA	Journal of the Chemical Society (A), Inorganic, Physical, Theoretical
JCSC	Journal of the Chemical Society, Chemical Communications
JCSD	Journal of the Chemical Society, Dalton Transactions
JCSF	Journal of the Chemical Society, Faraday Transactions
JECS	Journal of the European Ceramic Society
JIHU	Jiegou Huaxue, Chinese Journal of Structural Chemistry
JIP	Journal of Inclusion Phenomena
JIPC	Journal of Inclusion Phenomena and Macrocyclic Chemistry
JIPM	Journal of Inclusion Phenomena and Molecular Recognition in Chemistry
JJAP	Japanese Journal of Applied Physics
JKCS	Journal of the Korean Chemical Society
JKPS	Journal of the Korean Physical Society
JMC	Journal of Materials Chemistry
JMPS	Journal of Mineralogical and Petrological Sciences
JMR	Journal of Materials Research
JMRE	Journal of Magnetic Resonance
JPC	Journal Physical Chemistry
JPCB	Journal of Physical Chemistry, B
JPCC	Journal of Physical Chemistry, C
JPCM	Journal of Physics: Condensed Matter
JPCS	Journal of Physics and Chemistry of Solids
JPM	Journal of Porous Materials
JPSJ	Journal of the Physical Society of Japan

JPSS	Journal of Physics C: Solid State Physics
JRNC	Journal of Radioanalytical and Nuclear Chemistry
JSC	Journal of Structural Chemistry
JSIX	Journal of Surface Investigation, Synchrotron and Neutron Techniques
JSSC	Journal of Solid State Chemistry
KJC	Korean Journal of Crystallography
KT	Kristall und Technik
LAKS	Latvijas PSR Zinatnu Akademijas Vestis, Khimijas Serija
LANG	Langmuir
MCP	Materials Chemistry and Physics
MHCH	Monatshefte fuer Chemie
MIMA	Microporous Materials
MIMM	Microporous and Mesoporous Materials
MIZH	Mineralogicheskii Zhurnal
MJ	Mineralogical Journal
MM	Mineralogical Magazine
MOSI	Molecular Sieves, Synthesis of Microporous Materials, vol. 1
MP	Mineralogy and Petrology
MPA	Mineralogica Petrologica Acta
MRB	Materials Research Bulletin
MRSS	Materials Research Society Symposium Proceedings
MSEA	Materials Science and Engineering A - Structural Materials
MSF	Materials Science Forum
MSMS	Modelling and Simulation in Materials Science and Engineering
NANO	Nano Letters
NAT3	NATO ASI Series 3, High Technology
NATC	Nature Communications
NATM	Nature Materials
NATU	Nature
NATZ	Natural Zeolites, Pergamon, 1978, eds. L. B. Sand and F. A. Mumpton
NAWI	Naturwissenschaften
NGT	Norsk Geologisk Tidsskrift
NJC	New Journal of Chemistry
NJMA	Neues Jahrbuch fur Mineralogie, Abhandlungen
NJMM	Neues Jahrbuch fur Mineralogie, Monatshefte
NZTM	Natural Zeolites for the Third Millenium
OC	Original Contribution
P3ZC	Proceedings of the 3rd International Conference on Molecular Sieves
P5ZC	Proceedings of the 5th International Zeolite Conference
P6ZC	Proceedings of the 6th International Zeolite Conference
P7ZP	Preprints of Poster Papers, 7th International Zeolite Conference
P9ZC	Proceedings of the 9th International Zeolite Conference
P10Z	Proceedings of the 10th International Zeolite Conference
P12Z	Proceedings of the 12th International Zeolite Conference
P13Z	Proc. 13th Intern. Zeol. Conf., CD-ROM (quoted by chapter and number)
P14Z	Proc. 14th Intern. Zeol. Conf., CD-ROM
PC	Private communication
PCCP	Physical Chemistry Chemical Physics
PCG	Physics and Chemistry of Glasses
PCM	Physics and Chemistry of Minerals
PCTT	Physical Chemistry 2000, Proc. 5th Intern. Conf. Fund. & Appl. Asp. Phys. Chem.
PD	Powder Diffraction
PDAN	Physics, Doklady
PHYB	Physica B
PIAJ	Proceedngs of the Imperial Academy of Japan
PM	Periodico di Mineralogia
PNAS	Proceedings of the National Academy of Sciences
PRAA	Proceedings of the Royal Academy, Amsterdam
PRB	Physical Review B
PRSL	Proceedings of the Royal Society, London
PSTM	Publications Scientifiques et Techniques du Ministere de l'Air
RCM	Revue de Chimie minerale

RFP	Reactive and Functional Polymers
RHPS	Review of High Pressure Science and Technology, Kyoto
RIJO	Rigaku Journal
RJIC	Russian Journal of Inorganic Chemistry
RKHW	Rikogaku Kenkyusho Hokoku Waseda Daigaku
RLHX	Ran Liao Hua Xue Xue Bao, Taiwan
RP5Z	Recent Progress Reports and Discussion, 5th International Zeolite Conf., 1980
RP8Z	Recent Research Reports, 8th International Zeolite Conference, Amsterdam 1989
RRC	Revue Roumaine de Chimie
RSIM	Rendiconti Soc. Italiana di Mineralogia e Petrologia
R12Z	Recent Progress Reports, 12th International Zeolite Conference, Baltimore, 1998
R14Z	Recent Research Reports, 14th International Zeolite Conference, Cape Town 2004
SB	Structure and Bonding
SCI	Science
SCTE	Solid Compounds of Transition Elements, Intern. Conference, Stuttgart, 1979
SGWZ	Second German Workshop on Zeolite Chemistry
SILI	Silikaty
SPC	Soviet Physics, Crystallography
SPD	Soviet Physics, Doklady
SPSS	Soviet Physics, Solid State
SPUT	Scientific Papers of the College of General Education, University Tokyo
SSC	Solid State Communications
SSI	Solid State Ionics
SSS	Solid State Science
SSSC	Studies in Surface Science and Catalysis
SUMC	Supramolecular Chemistry
SXAP	Shiyu Xuebao (Acta Petrolei Sinica)
TFS	Transactions of the Faraday Society
TMPM	Tschermaks Mineralogisch-Petrographische Mitteilungen
VMUG	Vestnik Moskovskogo Universiteta, Seria 4, Geologiya
WHX	Wuji Huaxue Xuebao (Chinese Journal of Inorganic Chemistry)
XBNS	X-sen Bunseki no Shinpo (Advances in X-ray Chemical Analysis, Japan)
YKS	Yogyo-Kyokai-Shi
ZAAC	Zeitschrift fur Anorganische und Allgemeine Chemie
ZE97	Zeolites'97
ZEOL	Zeolites
ZNK	Zhurnal Neorganicheskoi Khimii
ZK	Zeitschrift fur Kristallographie
ZKNC	Zeitschrift fur Kristallographie, New Crystal Structures
ZKS	Zeitschrift fur Kristallographie, Supplement
ZNA	Zeitschrift fur Naturforschung, A
ZNB	Zeitschrift fur Naturforschung, B
ZVMO	Zapiski Vsesoyuznogo Mineralogicheskogo Obshchestva

5.2 Hot keys (shortcuts)

Database

Select new working directory	Ctrl+N
Open existing working directory	Ctrl+O
Exit	F10

Retrieve

Framework-type code (FTC)	Ctrl+Alt+F
Zeolite name	Ctrl+Alt+N
Bibliographic data	Ctrl+Alt+B
Key words	Ctrl+Alt+K
Chemical composition	Ctrl+Alt+C
Unit-cell parameters	Ctrl+Alt+U
Framework density	Ctrl+Alt+D
Symmetry	Ctrl+Alt+S
Distances and angles	Ctrl+Alt+A
Crystal system	Ctrl+Alt+R
temperature and pressure	Ctrl+Alt+T

Edit/view

Bibliographic data	Ctrl+B
Crystal data	Ctrl+D
Lattice parameters	Ctrl+L
Atomic coordinates	Ctrl+A
Atomic coordinates HTML	Ctrl+H
Sample data	Ctrl+M
Comments	Ctrl+T
TO-distances	Ctrl+O
TO-distances HTML table	Ctrl+I
ZeoBase.out	Ctrl+Z

Tools

Distances and angles	F2
SADIAN	F3
STRUPLO	F4
Powder pattern	F5
BRASS	F6

Export

cif	Ctrl+F
SADIAN	Ctrl+N
STRUPLO	Ctrl+R
Save active frame	Ctrl+S

Print

Print active frame	Ctrl+P
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Help

F1	not active yet
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5.3 File assignments

The following files are expected in three separate directories. It is assumed that the name of the directory where the program is installed is “zeobase”. “Anydir” is the name of the directory assigned upon clicking the open icon.

zeobase	zeobasedatabase⁺	anydir⁺⁺
zeobase_*.exe ⁺	*.bib entries	sad.inp SADIAN input
struplo.exe ⁺	*.xyz atomic coordinates	ZB_riet.cif cif for BRASS input
sadian.exe ⁺	*.sta standard coordinates	struplo.str STRUPLO input
rietveld.exe ⁺	zeobase.lin lines in list of selections	zeobase.out general output
riet.dll ⁺	zeolink control file	zeobase.cif cif export
rietcontrol.dll ⁺	zeobase.ind index file	zeograph.out data for XY and histogram
	journal.bin journal file	
	zeobase.rem remarks file	

⁺ programs and data files are expected on this directory

⁺⁺ output files are written to this directory